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A Gas-Kinetic Unified Algorithm for Non-Equilibrium Polyatomic Gas Flows Covering Various Flow Regimes

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Abstract. In this paper, a gas-kinetic unified algorithm (GKUA) is developed to investigate the non-equilibrium polyatomic gas flows covering various regimes. Based on the ellipsoidal statistical model with rotational energy excitation, the computable modelling equation is presented by unifying expressions on the molecular collision relaxing parameter and the local equilibrium distribution function. By constructing the corresponding conservative discrete velocity ordinate method for this model, the conservative properties during the collision procedure are preserved at the discrete level by the numerical method, decreasing the computational storage and time. Explicit and implicit lower-upper symmetric Gauss-Seidel schemes are constructed to solve the discrete hyperbolic conservation equations directly. Applying the new GKUA, some numerical examples are simulated, including the Sod Riemann problem, homogeneous flow rotational relaxation, normal shock structure, Fourier and Couette flows, supersonic flows past a circular cylinder, and hypersonic flow around a plate placed normally. The results obtained by the analytic, experimental, direct simulation Monte Carlo method, and other measurements in references are compared with the GKUA results, which are in good agreement, demonstrating the high accuracy of the present algorithm. Especially, some polyatomic gas non-equilibrium phenomena are observed and analysed by solving the Boltzmann-type velocity distribution function equation covering various flow regimes.

AMS subject classifications: 35Q20, 76P05, 82C40

Key words: Gas-kinetic unified algorithm, polyatomic gas, ellipsoidal statistical model, conservative discrete velocity ordinate method, implicit scheme.

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Nomenclature

α	energy-dependent deflection-angle exponent
β and θ	introduced relaxation parameter
δ	non-translational DoF of the gas
η	accommodation coefficient of solid wall
λ	mean free path
ν	collision frequency
σ and ζ	discrete velocity indexes in the V_x- and V_y-direction
τ	viscous stress tensor
χ	temperature exponent of the coefficient of viscosity
ω	index of the VHS model
A	weight of numerical quadrature rule
e_{tr} and e_{rot}	energies of translational motion and rotational structure
E	total energy
f	gas molecular velocity distribution function
f^{ES}	equilibrium distribution function
f_0	gas particle distribution in the $(\vec{\mathbf{r}},\vec{\mathbf{V}})$ phase space
f_1	the rotational energy density distribution
I	internal energy parameter
k	Boltzmann constant
m	gas molecular mass
n	particle number density
P	pressure
Pr	Prandtl number
R	gas constant
T_{ov}, T_{tr}, T_{rot} and T_{rel}	overall, translational, rotational and relaxation temperature
Z	rotational collision number
$\mathbf{\Theta}$	opposite of the stress tensor
$\mathcal{T}$	corrected tensor
$\overrightarrow{\mathbf{q_{tr}}}$, $\overrightarrow{\mathbf{q_{rot}}}$ and $\vec{\mathbf{q}}$	translational, rotational and total heat flux vector
$\vec{\mathbf{r}}=(x,y,z)^T$	space position vector
$\vec{\mathbf{U}}=(U,V,W)^T$	flow velocity vector
$\vec{\mathbf{V}}=(V_x,V_y,V_z)^T$	molecular velocity vector

1 Introduction

During spacecraft re-entry into atmosphere, various flow regimes can be confronted, e.g., the free molecule flow, rarefied transitional flow, slip and continuum flow regimes [1], where the thermodynamic properties of the gases and the non-equilibrium mechanism